Stability of Atoms in the Brown–Ravenhall Model

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Abstract

We consider the Brown–Ravenhall model of a relativistic atom with N electrons and a nucleus of charge Z and prove the existence of an infinite number of discrete eigenvalues for $N \leqslant Z$. As an intermediate result we prove a HVZ–type theorem for these systems.

1 Introduction

A fundamental fact of quantum mechanics is that any stable state (a state which can exist infinitely long in time) of a quantum system corresponds to an eigenfunction of the Hamiltonian of this system. In particular, for an atom, which is known to be a stable system, this means that its lowest spectral point should be an eigenvalue. Hence the existence of an eigenvalue at the bottom of the spectrum of the Hamiltonian can be considered as one of the criteria of correctness of a mathematical model of an atom.

For multiparticle Schrödinger operators on the mathematically rigorous level the existence of discrete eigenvalues at the bottom of the spectrum was proved by T. Kato (for an atom with two electrons) [13] and G. Zhislin (in the general case) [27]. In the following 45 years these results were generalized in many different directions. The existence of ground states was proved for atoms in an external magnetic field (J. Avron, I. Herbst, B. Simon [2] and S. Vugalter, G. Zhislin [23]), for the Herbst operator (S. Vugalter, G. Zhislin [26]). The most recent development is the proof of the existence of a stable ground state in the Pauli–Fierz model, which describes an atom interacting with a quantized radiation field (V. Bach, J. Fröhlich, I. Sigal [3]; J.–M. Barbaroux, T. Chen, S. Vugalter [5]; E. Lieb, M. Loss [16]).

In the work at hand we prove the existence of an infinite number of discrete eigenvalues, which accumulate at the bottom of the essential spectrum for the Brown–Ravenhall model of an atom or a positive atomic ion. The Brown–Ravenhall operator is one of the models used by physicists and quantum–chemists to describe relativistic effects in atoms (for a discussion of physical accuracy of this model see [18]).

The mathematically rigorous study of this operator started with the work by W. Evans, P. Perry and H. Siedentop [7], who proved that the Brown–Ravenhall operator of a one–particle Coulomb system with the nuclear charge Z is semibounded from below for $\alpha Z \leqslant 2\left(\frac{\pi}{2}+\frac{2}{\pi}\right)^{-1}$, where α is the fine structure constant. Further results on the lower bound of the spectrum of this operator with one electron and one or several nuclei were obtained by C. Tix [20, 21] and A. Balinsky, W. Evans [4].

Although the questions of semiboundedness and self–adjointness of the Brown–Ravenhall operator are extremely important, its successful application requires much more detailed knowledge of its spectral properties. The goal of this paper is to establish some of them.

A way to prove the existence of a stable ground state of a multiparticle system was developed by G. Zhislin in [27] and consists of two steps. The first step is to prove a so–called HVZ–type theorem which establishes a criterion for the existence of a bound state. The second step is a construction of a trial function which satisfies this criterion. In the work at hand we follow the same strategy. First we prove a HVZ–type theorem (Theorem 1), showing that the bottom of the essential spectrum of the Brown–Ravenhall operator of an atomic system with N electrons is determined by the bottom of the spectrum of the operator with $N-1$ electrons. Then we construct a trial function with an expectation value of the energy less than the bottom of the essential spectrum (Theorem 2). Although we use the same strategy as in the original paper by G. Zhislin, the work at hand is technically very different from the works on Schrödinger operators. The main differences are caused by the nonlocality of the Brown–Ravenhall operator. Notice that the HVZ theorem was proved earlier by R. Lewis, H. Siedentop and S. Vugalter [15] for the Herbst–type operator, which is also non–local. The Brown–Ravenhall operator in contrast to the Herbst operator has, however, not only a non–local kinetic energy, but also a non–local potential energy. This leads to a large number of additional complications.

In Section 3 we prove several lemmata which allow us to estimate these non–local effects and to modify the method of [27] in such a way that it works also for the Brown–Ravenhall operator. Here the most important role is played by the estimates on the commutator of the projector on the positive spectral subspace of the Dirac operator with a smoothed characteristic function of a region in the configuration space (Lemma 1) and the decay of the integral kernel of this projector (Lemma 2).

When this work was in preparation, the authors received two preprints by D. Jakubaßa–Amundsen [12, 11], where the HVZ theorem for the Brown–Ravenhall operator was proved in a different way and without taking the Pauli principle into account.

2 Preliminaries

The N–electron Brown–Ravenhall Hamiltonian is given by

$$\mathcal{H}_N = \Lambda_+^N \left(\sum_{n=1}^{N} \left(D_n - \frac{\alpha Z}{|\mathbf{x}_n|} \right) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|} \right) \Lambda_+^N. \tag{2.1}$$

Here $\mathbf{x}_n \in \mathbb{R}^3$ is the position vector of the n^{th} electron. The Dirac operator in the standard representation is given by

$$D = -i\boldsymbol{\alpha} \cdot \nabla + \beta, \tag{2.2}$$

where $\boldsymbol{\alpha} := (\alpha_1, \alpha_2, \alpha_3)$ and β are the the four Dirac matrices, explicitly

$$\alpha_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}, \quad k = 1, 2, 3,$$

σ_k denoting the k^{th} Pauli matrix

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

and

$$\beta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

D_n is the Dirac operator D acting on the coordinates of the n^{th} electron. Z is the nuclear charge, $\alpha \approx 1/137$ is the fine structure constant, and

$$\Lambda_+^N = \bigotimes_{n=1}^{N} \Lambda_+^{(n)}, \tag{2.3}$$

where $\Lambda_+^{(n)}$ is the projector onto the positive spectral subspace of D_n.

The underliying Hilbert space is $\mathfrak{H}^N := \Lambda_+^N \bigwedge_{n=1}^{N} L_2(\mathbb{R}^3, \mathbb{C}^4)$, where $\wedge$ stands for the antisymmetric tensor product of one–electron Hilbert spaces. The operator $\mathcal{H}_N$ is well defined as the operator corresponding to the semibounded closed form on $\Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ for

$$\alpha Z < \alpha Z_c = \frac{2}{\left(\frac{\pi}{2} + \frac{2}{\pi}\right)}. \tag{2.4}$$

We always assume in the following that condition (2.4) is fulfilled.

The semiboundedness of $\mathcal{H}_N$ follows from the semiboundedness of the one–particle operators $\Lambda_+\Big(D - \frac{\alpha Z}{|\mathbf{x}|}\Big)\Lambda_+$ (see [7]) and the positivity of the two–particle interaction terms.

We denote the spectrum of an arbitrary selfadjoint operator A by $\sigma(A)$. $[A, B] = AB - BA$ is the commutator of two operators. $B(R, \mathbf{x})$ is the open ball in $\mathbb{R}^d$ of radius $R > 0$ centered at $\mathbf{x}$. $B(R) := B(R, \mathbf{0})$. $\langle\cdot,\cdot\rangle$ and $\|\cdot\|$ stand for the inner product and the norm in $L_2(\mathbb{R}^{3d}, \mathbb{C}^{4^d})$. d is usually clear by context. Let $E_{N-1} := \inf\sigma(\mathcal{H}_{N-1})$. Irrelevant constants are denoted by C. I_Ω is the indicator function of the set Ω. The Fourier transform of f is denoted by $\hat{f}$.

In auxiliary calculations it is sometimes convenient to consider the operator (2.1) in the space $\Lambda_+^N \overset{N}{\underset{n=1}{\otimes}} L_2(\mathbb{R}^3, \mathbb{C}^4)$, i. e. without antisymmetrization. We use this extension without changing the notation.

The main result of this article are the following two theorems.

Theorem 1 *For any $N > 1$, we have*

$$\sigma_{\mathrm{ess}}(\mathcal{H}_N) = [E_{N-1} + 1, \infty). \tag{2.5}$$

Theorem 2 *Let $N \leqslant Z$. Then the operator $\mathcal{H}_N$ has infinitely many eigenvalues below the essential spectrum.*

Remark 1 *Theorem 1 is an analogue of the HVZ theorem for multiparticle Schrödinger operators (see [6] and the original papers [27, 22, 10]). Analogous theorems were proved for the magnetic Schrödinger operator [24] and the Herbst operator [15].*

Remark 2 *In contrast to the Schrödinger case the bottom of the essential spectrum of $\mathcal{H}_N$ is $E_{N-1}+1$ and not E_N. This is related to the fact that in the Brown–Ravenhall model the spectrum of the free electron is $[1, \infty)$ instead of $[0, \infty)$.*

Remark 3 *In the multiparticle Schrödinger case the existence of discrete eigenvalues was proved in [13] for $N = 2$, and in [27] for arbitrary N.*

The proof of Theorem 1 is given in Sections 4 and 5. Theorem 2 is proved in Section 6. Section 3 contains some lemmata used in the subsequent sections.

3 Technical Lemmata

3.1 Commutator Estimate

The projector Λ_+ for the free one–particle Dirac operator is given by (see [19], formula 1.1.54)

$$\Lambda_+ = \frac{1}{2} + \frac{D}{2|D|} = \frac{1}{2} + \mathcal{F}^* \frac{\boldsymbol{\alpha}\cdot\mathbf{p} + \beta}{2\sqrt{|\mathbf{p}|^2 + 1}}\mathcal{F}, \tag{3.1}$$

where $\mathcal{F}$ is the Fourier transform. In the coordinate representation for $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ the operator Λ_+ acts as

$$(\Lambda_+ f)(\mathbf{x}) = \frac{f(\mathbf{x})}{2} + \frac{1}{4\pi^2} \int\limits_{\mathbb{R}^3} \left(\beta \frac{K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} + \frac{i\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2} K_0\big(|\mathbf{x}-\mathbf{y}|\big) \right) f(\mathbf{y}) d\mathbf{y}$$
$$+ \frac{i}{2\pi^2} \lim_{\varepsilon \to +0} \int\limits_{\mathbb{R}^3 \setminus B(\varepsilon, \mathbf{x})} \frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3} K_1\big(|\mathbf{x}-\mathbf{y}|\big) f(\mathbf{y}) d\mathbf{y}, \tag{3.2}$$

where the limit on the r. h. s. is the limit in $L_2(\mathbb{R}^3, \mathbb{C}^4)$ (see Appendix B). For convenience of the reader we state properties of the functions K_ν, $\nu = 1, 2$, in Appendix A.

Lemma 1 *Let $\chi \in C^2(\mathbb{R}^3)$. Then the norm of the operator*

$$[\chi, \Lambda_+] : L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^1(\mathbb{R}^3, \mathbb{C}^4)$$

satisfies

$$\big\|[\chi, \Lambda_+]\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to H^1(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C\big(\|\nabla\chi\|_\infty + \|\partial^2\chi\|_\infty\big). \tag{3.3}$$

Here $\|\partial^2\chi\|_\infty = \max\limits_{\substack{\mathbf{z}\in\mathbb{R}^3 \\ k,l\in\{1,2,3\}}} \big|\partial^2_{kl}\chi(\mathbf{z})\big|$.

In the proof of Lemma 1 we shall apply the following theorem, which we formulate here for convenience of the reader.

Theorem 3 (Stein [17], Chapter 2, sec. 3.2) *Let $K : \mathbb{R}^n \to \mathbb{C}$ be measurable such that*

$$\big|K(\mathbf{x})\big| \leqslant B|\mathbf{x}|^{-n}, \quad \mathbf{x} \neq \mathbf{0}, \tag{3.4}$$

$$\int\limits_{|\mathbf{x}|\geqslant 2|\mathbf{y}|} \big|K(\mathbf{x}-\mathbf{y}) - K(\mathbf{x})\big| d^n\mathbf{x} \leqslant B, \quad 0 < |\mathbf{y}|, \tag{3.5}$$

and

$$\int\limits_{R_1<|\mathbf{x}|<R_2} K(\mathbf{x}) d^n\mathbf{x} = 0, \quad \textit{for all} \quad 0 < R_1 < R_2 < \infty. \tag{3.6}$$

For an arbitrary $f \in L_p(\mathbb{R}^n)$, $1 < p < \infty$, let

$$T_\varepsilon(f)(\mathbf{x}) = \int\limits_{|\mathbf{y}|\geqslant\varepsilon} f(\mathbf{x}-\mathbf{y}) K(\mathbf{y}) d^n\mathbf{y}, \quad \varepsilon > 0. \tag{3.7}$$

Then

$$\big\|T_\varepsilon(f)\big\|_p \leqslant A_p\|f\|_p \tag{3.8}$$

with A_p independent of f and ε.

Remark 4 *Inequality* (3.8) *shows that the operator* $T = \lim_{\varepsilon\to+0} T_\varepsilon$ *exists as a bounded operator in* $L_p(\mathbb{R}^n)$ *and its norm satisfies* $\|T\|_p \leqslant A_p$.

Proof of Lemma 1. Let us first prove that $[\chi, \Lambda_+]$ is a bounded operator in $L_2(\mathbb{R}^3, \mathbb{C}^4)$. For $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ formula (3.2) implies

$$\begin{aligned}
&\big([\chi, \Lambda_+]f\big)(\mathbf{x}) \\
&= \frac{1}{4\pi^2}\int \left(\beta \frac{K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|} + \frac{i\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}K_0\big(|\mathbf{x}-\mathbf{y}|\big)\right)\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y} \\
&\qquad + \frac{i}{2\pi^2}\int \frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^3}K_1\big(|\mathbf{x}-\mathbf{y}|\big)\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}.
\end{aligned} \tag{3.9}$$

Estimating $\big|\chi(\mathbf{x})-\chi(\mathbf{y})\big|$ by $|\mathbf{x}-\mathbf{y}|\|\nabla\chi\|_\infty$, using the density of $C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ in $L_2(\mathbb{R}^3, \mathbb{C}^4)$ and applying the Young inequality for the convolution with a kernel from $L_1(\mathbb{R}^3)$, we arrive at

$$\begin{aligned}
&\big\|[\chi, \Lambda_+]\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to L_2(\mathbb{R}^3,\mathbb{C}^4)} \\
&\leqslant \|\nabla\chi\|_\infty \frac{1}{4\pi^2}\int \left(K_1\big(|\mathbf{x}|\big) + 3K_0\big(|\mathbf{x}|\big) + 6\frac{K_1\big(|\mathbf{x}|\big)}{|\mathbf{x}|}\right)d\mathbf{x} \leqslant C\|\nabla\chi\|_\infty.
\end{aligned} \tag{3.10}$$

To complete the proof of Lemma 1 one has to show that

$$\big\|\nabla[\chi, \Lambda_+]f\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)} \leqslant C\big(\|\nabla\chi\|_\infty + \|\partial^2\chi\|_\infty\big)\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}.$$

The differentiation of the first summand on the r. h. s. of (3.9) gives absolutely convergent integrals whose L_2–norms are bounded by $C\|\nabla\chi\|_\infty\|f\|$. The differentiation of the second integral on the r. h. s. of (3.9) in the j^{th} component of $\mathbf{x}$ gives for $f \in C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ (cf. Appendix B)

$$\begin{aligned}
&\frac{i}{2\pi^2}\lim_{\varepsilon\to+0}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)} \left(\alpha_j\frac{K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3} - \frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_0\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^4}\right. \\
&\qquad\qquad \left. - \frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^5}\right)\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y} \\
&\qquad + \frac{i}{2\pi^2}\lim_{\varepsilon\to+0}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)} \frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}\partial_j\chi(\mathbf{x})f(\mathbf{y})d\mathbf{y}.
\end{aligned} \tag{3.11}$$

The term

$$-\frac{i}{2\pi^2}\int \frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)K_0\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^4}\big(\chi(\mathbf{x})-\chi(\mathbf{y})\big)f(\mathbf{y})d\mathbf{y}$$

is bounded by $C\|\nabla\chi\|_\infty\|f\|$.

The Taylor expansion of χ gives

$$\chi(\mathbf{x})-\chi(\mathbf{y}) = (x_k-y_k)\partial_k\chi(\mathbf{x})-\frac{1}{2}(x_k-y_k)(x_l-y_l)\partial^2_{kl}\chi(\mathbf{z}_{xy}), \quad \mathbf{z}_{xy}\in[\mathbf{x},\mathbf{y}]. \tag{3.12}$$

Here $[\mathbf{x},\mathbf{y}]$ is the line segment connecting $\mathbf{x}$ and $\mathbf{y}$ and summations in k and l from 1 to 3 are assumed. Substituting (3.12) into (3.11) we arrive at

$$\begin{aligned}
&\frac{i\partial_k\chi(\mathbf{x})}{2\pi^2}\lim_{\varepsilon\to+0}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)}\left(\alpha_j-\frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^2}\right)\frac{K_1\big(|\mathbf{x}-\mathbf{y}|\big)(x_k-y_k)}{|\mathbf{x}-\mathbf{y}|^3}f(\mathbf{y})d\mathbf{y}\\
&\quad+\frac{i\partial_j\chi(\mathbf{x})}{2\pi^2}\lim_{\varepsilon\to+0}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)}\frac{\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}f(\mathbf{y})d\mathbf{y}\\
&\qquad-\frac{i}{4\pi^2}\int\left(\alpha_j-\frac{4\boldsymbol{\alpha}\cdot(\mathbf{x}-\mathbf{y})(x_j-y_j)}{|\mathbf{x}-\mathbf{y}|^2}\right)\frac{K_1\big(|\mathbf{x}-\mathbf{y}|\big)}{|\mathbf{x}-\mathbf{y}|^3}\\
&\qquad\qquad\times(x_k-y_k)(x_l-y_l)\partial^2_{kl}\chi(\mathbf{z}_{xy})f(\mathbf{y})d\mathbf{y}.
\end{aligned} \tag{3.13}$$

To the first two integrals in (3.13) we shall apply Theorem 3 with $n=3$. Hypotheses (3.4) and (3.6) are obviously fulfilled. To prove that condition (3.5) is also fulfilled we note that (3.5) follows from the estimate

$$\big|\nabla K(\mathbf{x})\big|\leqslant B|\mathbf{x}|^{-4} \tag{3.14}$$

(see [17], page 34). Inequality (3.14) follows from (A.2). Due to Theorem 3 the L_2–norms of the first two integrals in (3.13) are bounded by $C\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}$. The last term in (3.13) is a convolution with a function from $L_1(\mathbb{R}^3)$, whose L_2–norm due to the Young inequality can be estimated with

$$C\|\partial^2\chi\|_\infty\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}.$$

This completes the proof of Lemma 1. •

3.2 Non–local Properties of the Operator Λ_+

Lemma 2 *Let* $\mathrm{supp}f\subset\Omega\subset\mathbb{R}^3$, $|\Omega|<\infty$, $\mathbf{x}\in\mathbb{R}^3$, $d:=\mathrm{dist}(\mathbf{x},\Omega)>0$. *Then*

$$\big|(\Lambda_+f)(\mathbf{x})\big|\leqslant G(d)|\Omega|^{1/2}\|f\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}, \tag{3.15}$$

where

$$G(d)=\frac{1}{4\pi^2}\Big(\frac{K_1(d)}{d}+3\frac{K_0(d)}{d}+6\frac{K_1(d)}{d^2}\Big). \tag{3.16}$$

Proof. The statement of Lemma 2 follows immediately from the Schwarz inequality and formula (3.2), if we note that for $\mathbf{x}\notin\mathrm{supp}\,f$ all integrals in (3.2) converge absolutely. •

Remark 5 *Notice that the functions $K_\nu(d)$, $\nu = 0, 1$, and consequently $G(d)$, decay exponentially according to* (A.1) *as $d \to \infty$. Our proof of the HVZ theorem and of the existence of the discrete spectrum follows the same lines as in the original paper by G. Zhislin [27] for the Schrödinger operator. The new obstacle which was overcome in the present work is the non–locality of the Brown–Ravenhall operator. Lemma 2 tells us that, although the operator Λ_+ is non–local, for a compactly supported function f the function $\Lambda_+ f$ decays exponentially with the distance to the support of f.*

3.3 Localization Error Estimate

Lemma 3 *Any bounded function $\chi \in C^1(\mathbb{R}^d)$ with bounded derivatives is a multiplicator in $H^{1/2}(\mathbb{R}^d, \mathbb{C}^k)$ for any $d, k \in \mathbb{N}$:*

$$\|\chi u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} \leqslant C_d \cdot \big(\|\chi\|_{L_\infty(\mathbb{R}^d)} + \|\nabla\chi\|_{L_\infty(\mathbb{R}^d)}\big)\|u\|_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)}, \tag{3.17}$$

for all $u \in H^{1/2}(\mathbb{R}^d, \mathbb{C}^k)$.

Proof of Lemma 3. We choose the norm in $H^{1/2}(\mathbb{R}^d, \mathbb{C}^k)$ as (see [1], Theorem 7.48).

$$\|u\|^2_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} := \|u\|^2_{L_2(\mathbb{R}^d,\mathbb{C}^k)} + \iint \frac{\big|u(\mathbf{x}) - u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} d\mathbf{y}. \tag{3.18}$$

Then

$$\begin{aligned} \|\chi u\|^2_{H^{1/2}(\mathbb{R}^d,\mathbb{C}^k)} &= \|\chi u\|^2_{L_2(\mathbb{R}^d,\mathbb{C}^k)} + \iint \frac{\big|\chi(\mathbf{x})u(\mathbf{x}) - \chi(\mathbf{y})u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} d\mathbf{y} \\ \leqslant \|\chi\|^2_{L_\infty}\|u\|^2_{L_2} &+ \iint \left(\frac{\big|\chi(\mathbf{x})\big|^2\big|u(\mathbf{x}) - u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} + \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2\big|u(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} \right) d\mathbf{x} d\mathbf{y} \\ &\leqslant \|\chi\|^2_{L_\infty}\|u\|^2_{H^{1/2}} + \sup_{\mathbf{y}\in\mathbb{R}^d} \int \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} \|u\|^2_{L_2}. \end{aligned} \tag{3.19}$$

The supremum on the r. h. s. of (3.19) can be estimated as

$$\begin{aligned} \sup_{\mathbf{y}\in\mathbb{R}^d} \int \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} &\leqslant \sup_{\mathbf{y}\in\mathbb{R}^d} \int_{B(1,\mathbf{y})} \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} \\ + \sup_{\mathbf{y}\in\mathbb{R}^d} \int_{\mathbb{R}^d\setminus B(1,\mathbf{y})} \frac{\big|\chi(\mathbf{x}) - \chi(\mathbf{y})\big|^2}{|\mathbf{x}-\mathbf{y}|^{d+1}} d\mathbf{x} &\leqslant |S_{d-1}|\big(\|\nabla\chi\|^2_{L_\infty} + 4\|\chi\|^2_{L_\infty}\big), \end{aligned} \tag{3.20}$$

where $|S_{d-1}|$ is the area of $(d-1)$–dimensional unit sphere. Substituting (3.20) into (3.19) and using the inequality $a^2 + b^2 \leqslant (a+b)^2$ for $a, b \geqslant 0$ we obtain (3.17). •

Lemma 4 *For any bounded function $\chi \in C^1(\mathbb{R}^{3N})$ with bounded derivatives the operator $[\chi, \Lambda_+^N]$ is bounded in $H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ and for any $\psi \in H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ we have*

$$\begin{aligned}&\big\|[\chi, \Lambda_+^N]\psi\big\|_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\\ &\leqslant C_N\big(\|\nabla\chi\|_{L_\infty(\mathbb{R}^{3N})} + \|\partial^2\chi\|_{L_\infty(\mathbb{R}^{3N})}\big)\big(1 + \|\nabla\chi\|_{L_\infty(\mathbb{R}^{3N})}\big)\|\psi\|_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}.\end{aligned} \tag{3.21}$$

Proof. Successively commuting χ with one–particle projections $\Lambda_+^{(n)}$, $n = 1, \dots, N$ (see (2.3)) we obtain

$$[\chi, \Lambda_+^N] = \sum_{n=1}^{N}\prod_{k=1}^{n-1}\Lambda_+^{(k)}[\chi, \Lambda_+^{(n)}]\prod_{l=n+1}^{N}\Lambda_+^{(l)}, \tag{3.22}$$

where the empty products should be replaced by identity operators. According to (3.1), the operator Λ_+ is bounded in $H^s(\mathbb{R}^3, \mathbb{C}^4)$ for any $s \in \mathbb{R}$. This, together with (3.22), and Lemmata 1 and 3, implies (3.21). •

Lemma 5 *There exists a constant $C_{N,Z}$ depending on N and Z such that for any $\psi \in \Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$*

$$\langle \mathcal{H}_N\psi, \psi\rangle \geqslant C_{N,Z}\|\psi\|^2_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}. \tag{3.23}$$

Proof. For the one particle Brown–Ravenhall operator one has (see [21])

$$\Lambda_+\Big(D - \frac{\alpha Z}{|\mathbf{x}|}\Big)\Lambda_+ \geqslant (1 - \alpha Z)\Lambda_+. \tag{3.24}$$

Inequality (3.24) holds true for any $Z \leqslant Z_c$ (cf. (2.4)). Using (3.24) with $Z = Z_c$ we get

$$\Lambda_+\Big(D - \frac{\alpha Z}{|\mathbf{x}|}\Big)\Lambda_+ \geqslant \frac{Z_c - Z}{Z_c}D\Lambda_+ + \frac{Z}{Z_c}(1 - \alpha Z_c)\Lambda_+ \geqslant \frac{Z_c - Z}{Z_c}D\Lambda_+. \tag{3.25}$$

Now, since $\sum_{n<j}^{N} \dfrac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|} > 0$, $Z < Z_c$, and $\psi = \Lambda_+^N\psi$, using (3.25) we obtain

$$\langle \mathcal{H}_N\psi, \psi\rangle \geqslant \langle\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big)\psi, \psi\rangle \geqslant C_Z\langle\sum_{n=1}^{N}D_n\psi, \psi\rangle \geqslant C_{N,Z}\|\psi\|^2_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})}, \tag{3.26}$$

which is (3.23) •

Lemma 6 *Let $\{\chi_a\}_{a\in\mathcal{A}}$ be a partition of unity with the properties*

$$\chi_a \in C^2(\mathbb{R}^{3N}), \quad \chi_a \geqslant 0, \quad \sum_{a\in\mathcal{A}} \chi_a^2 = 1. \tag{3.27}$$

Then for any $\psi \in \Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ we have

$$\begin{aligned}&\Big|\langle \mathcal{H}_N \psi, \psi\rangle - \sum_{a\in\mathcal{A}} \langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi\rangle\Big|\\ &\leqslant \widetilde{C}_{N,Z} \sum_{a\in\mathcal{A}} \big(\|\nabla\chi_a\|_{L_\infty(\mathbb{R}^{3N})} + \|\partial^2\chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)\big(1 + \|\nabla\chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)^2 \langle \mathcal{H}_N \psi, \psi\rangle.\end{aligned} \tag{3.28}$$

Proof. We write

$$\begin{aligned}\langle \mathcal{H}_N \psi, \psi\rangle &= \Big\langle \Big(\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|}\Big) \sum_{a\in\mathcal{A}} \chi_a^2 \Lambda_+^N \psi, \Lambda_+^N \psi\Big\rangle\\ &= \sum_{a\in\mathcal{A}} \Big\langle \Big(\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|}\Big) \chi_a \Lambda_+^N \psi, \chi_a \Lambda_+^N \psi\Big\rangle\\ &= \sum_{a\in\mathcal{A}} \langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi\rangle\\ &+ \sum_{a\in\mathcal{A}} \Big\langle \Big(\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|}\Big) [\chi_a, \Lambda_+^N] \psi, \chi_a \Lambda_+^N \psi\Big\rangle\\ &+ \sum_{a\in\mathcal{A}} \Big\langle \Lambda_+^N \chi_a \psi, \Big(\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|}\Big) [\chi_a, \Lambda_+^N] \psi\Big\rangle.\end{aligned} \tag{3.29}$$

In the second line of (3.29) we used the relation

$$\sum_{a\in\mathcal{A}} \langle g, \nabla(\chi_a^2 g)\rangle = \sum_{a\in\mathcal{A}} \langle \chi_a g, \nabla(\chi_a g)\rangle + \sum_{a\in\mathcal{A}} \langle g, \nabla\Big(\frac{\chi_a^2}{2}\Big) g\rangle, \tag{3.30}$$

which holds for any $g \in H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. The last term in (3.30) is zero because of (3.27).

It remains to estimate the last two terms on the r. h. s. of (3.29). Since the sesquilinear form of $\sum_{n=1}^{N}\Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|}\Big) + \sum_{n<j}^{N} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_j|}$ is bounded on $H^{1/2}(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ (for the potential energy terms this follows from the Kato inequality), Lemmata 3

and 4 imply that

$$\Big|\langle\Big(\sum_{n=1}^{N}\Big(D_n-\frac{\alpha Z}{|\mathbf{x}_n|}\Big)+\sum_{n<j}^{N}\frac{\alpha}{|\mathbf{x}_n-\mathbf{x}_j|}\Big)[\chi_a,\Lambda_+^N]\psi,\chi_a\Lambda_+^N\psi\rangle$$

$$+\langle\Lambda_+^N\chi_a\psi,\Big(\sum_{n=1}^{N}\Big(D_n-\frac{\alpha Z}{|\mathbf{x}_n|}\Big)+\sum_{n<j}^{N}\frac{\alpha}{|\mathbf{x}_n-\mathbf{x}_j|}\Big)[\chi_a,\Lambda_+^N]\psi\rangle\Big| \tag{3.31}$$

$$\leqslant \widetilde{C}_{N,Z}\big(\|\nabla\chi_a\|_{L_\infty(\mathbb{R}^{3N})}+\|\partial^2\chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)$$
$$\times\big(1+\|\nabla\chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)^2\|\psi\|^2_{H^{1/2}(\mathbb{R}^{3N},\mathbb{C}^{4^N})},\quad \text{for all}\quad a\in\mathcal{A}.$$

The relation (3.28) follows from (3.29), (3.31) and Lemma 5. •

4 Proof of Theorem 1: "Easy Part"

We shall prove that

$$\sigma_{\mathrm{ess}}(\mathcal{H}_N)\supseteq[E_{N-1}+1,\infty), \tag{4.1}$$

by construction of an appropriate Weyl sequence for $\mathcal{H}_N$ at the point $E_{N-1}+\lambda$ for any $\lambda\geqslant 1$.

Since $\mathcal{H}_N$ commutes with the projector P_A onto the antisymmetric subspace, it suffices to find a Weyl sequence $\{\Psi_l\}_{l=1}^{\infty}\in\bigotimes_{n=1}^{N}L_2(\mathbb{R}^3,\mathbb{C}^4)$ such that for l big enough

$$\|P_A\Psi_l\|>\delta_0,\quad \delta_0>0, \tag{4.2}$$

where δ_0 is independent of l.

For $j\in\mathbb{N}$ let

$$\varphi_j\in P_{[E_{N-1},E_{N-1}+j^{-1})}(\mathcal{H}_{N-1})\mathfrak{H}^{N-1},\quad \|\varphi_j\|_{L_2(\mathbb{R}^{3(N-1)},\mathbb{C}^{4^{(N-1)}})}=1. \tag{4.3}$$

Here $P_J(\mathcal{H}_{N-1})$ is the spectral projector of $\mathcal{H}_{N-1}$ corresponding to the interval J.

We choose a vector $\mathbf{k}\in\mathbb{R}^3$ with

$$\sqrt{1+|\mathbf{k}|^2}=\lambda. \tag{4.4}$$

Let $\chi\in C_0^\infty(\mathbb{R}^3)$ be a function with $\operatorname{supp}\chi\subset\big\{\mathbf{y}\in\mathbb{R}^3\,\big|\,1\leqslant|\mathbf{y}|\leqslant 2\big\}$, $\|\chi\|_{L_2(\mathbb{R}^3)}=1$. For $\mathbf{p}\in\mathbb{R}^3$ we define a family of operators $\Lambda_+(\mathbf{p})$ in $\mathbb{C}^4$ by

$$\Lambda_+(\mathbf{p}):=\frac{1}{2}+\frac{\boldsymbol{\alpha}\cdot\mathbf{p}+\beta}{2\sqrt{|\mathbf{p}|^2+1}}. \tag{4.5}$$

Let $u(\mathbf{k})\in\operatorname{Ran}\big(\Lambda_+(\mathbf{k})\big)$ and $\big|u(\mathbf{k})\big|=1$. Then (4.4) implies

$$(\boldsymbol{\alpha}\cdot\mathbf{k}+\beta)u(\mathbf{k})=\lambda u(\mathbf{k}). \tag{4.6}$$

For a sequence $0 < R_j \nearrow \infty,\ j \in \mathbb{N}$ we define

$$\psi_j(\mathbf{y}) := R_j^{-3/2} \chi(R_j^{-1}\mathbf{y}) e^{i\mathbf{k}\cdot\mathbf{y}} u(\mathbf{k}), \quad \mathbf{y} \in \mathbb{R}^3, \quad j \in \mathbb{N}. \tag{4.7}$$

Assuming that

$$R_{j+1} \geqslant 2R_j, \tag{4.8}$$

we get

$$\langle \psi_j, \psi_k \rangle = \delta_{jk}, \quad j, k \in \mathbb{N}. \tag{4.9}$$

Lemma 7 *For the sequence $\{\psi_j\}_{j=1}^{\infty}$ we have*

$$\|\Lambda_+ \psi_j - \psi_j\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \underset{j\to\infty}{\longrightarrow} 0. \tag{4.10}$$

Proof. Since the Fourier transform of ψ_j is

$$\hat{\psi}_j(\mathbf{p}) = R_j^{3/2} \hat{\chi}\big(R_j(\mathbf{p} - \mathbf{k})\big) u(\mathbf{k}),$$

one has

$$\begin{aligned} &\|\Lambda_+ \psi_j - \psi_j\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \\ &\quad \leqslant \Big\| \big(\Lambda_+(\mathbf{p}) - 1\big) I_{B(R_j^{-1/2}, \mathbf{k})}(\mathbf{p}) R_j^{3/2} \hat{\chi}\big(R_j(\mathbf{p} - \mathbf{k})\big) u(\mathbf{k}) \Big\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)} \\ &\quad + \Big\| \big(\Lambda_+(\mathbf{p}) - 1\big) I_{\mathbb{R}^3 \setminus B(R_j^{-1/2}, \mathbf{k})}(\mathbf{p}) R_j^{3/2} \hat{\chi}\big(R_j(\mathbf{p} - \mathbf{k})\big) u(\mathbf{k}) \Big\|_{L_2(\mathbb{R}^3, \mathbb{C}^4)}. \end{aligned} \tag{4.11}$$

Obviously

$$\Big\| \big(\Lambda_+(\mathbf{p}) - 1\big) - \big(\Lambda_+(\mathbf{k}) - 1\big) \Big\|_{\mathbb{C}^4 \to \mathbb{C}^4} \leqslant C|\mathbf{p} - \mathbf{k}|$$

for $C > 0$ independent of $\mathbf{k}$. Hence one can estimate the first term in (4.11) by $CR_j^{-1/2}\|\chi\|_{L_2(\mathbb{R}^3)}$. The second term in (4.11) is bounded by $\|\hat{\chi}\|_{L_2(\mathbb{R}^3 \setminus B(R_j^{1/2}))}$, and consequently converges to zero, too. •

Now we are ready to define the desired Weyl sequence. Let

$$\begin{aligned} \Psi_j(\mathbf{x}, \mathbf{x}_N) : &= \varphi_j(\mathbf{x}) \otimes \psi_j(\mathbf{x}_N), \\ &\mathbf{x} = (\mathbf{x}_1, \dots, \mathbf{x}_{N-1}) \in \mathbb{R}^{3(N-1)}, \quad \mathbf{x}_N \in \mathbb{R}^3, \quad j \in \mathbb{N}. \end{aligned} \tag{4.12}$$

Recall that φ_j is a vector function with $4^{(N-1)}$ components and ψ_j is a vector function with 4 components.

Lemma 8 *The sequence $\{\Psi_j\}_{j=1}^{\infty}$ has the following properties:*

(i) $\|\Lambda_+^N \Psi_j\| \underset{j\to\infty}{\longrightarrow} 1,$

(ii) $|\langle \Lambda_+^N \Psi_j, \Lambda_+^N \Psi_k \rangle| \to 0, \quad k \neq j, \quad k, j \to \infty,$

$$\text{(iii)} \quad \big\|(\mathcal{H}_N - E_{N-1} - \lambda)\Lambda_+^N \Psi_j\big\| \underset{j\to\infty}{\longrightarrow} 0. \tag{4.13}$$

Proof of Lemma 8. Relations (i) and (ii) follow from Lemma 7 and relation (4.9).
Let us prove (4.13). We have

$$\begin{aligned}&(\mathcal{H}_N - E_{N-1} - \lambda)\Lambda_+^N \Psi_j \\ &= (\mathcal{H}_{N-1} - E_{N-1})\Lambda_+^N \Psi_j + \Lambda_+^N \biggl((D_N - \lambda) - \frac{\alpha Z}{|\mathbf{x}_N|} + \sum_{n=1}^{N-1} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_N|} \biggr) \Lambda_+^N \Psi_j.\end{aligned} \tag{4.14}$$

The operator $\mathcal{H}_{N-1}$ acts on the function φ_j only.
The first term in (4.14) tends to zero in norm according to (4.3).
Since Λ_+^N commutes with D_N we have

$$\begin{aligned}\bigl\|(D_N - \lambda)\Lambda_+^N \Psi_j\bigr\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})} &\leqslant \bigl\|(D_N - \lambda)\Psi_j\bigr\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})} \\ &\leqslant \bigl\|R_j^{-3/2} \boldsymbol{\alpha} \cdot \nabla_{\mathbf{x}_N} \chi(R_j^{-1}\mathbf{x}_N) u(\mathbf{k})\bigr\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)} \underset{j\to\infty}{\longrightarrow} 0.\end{aligned} \tag{4.15}$$

In the second inequality of (4.15) we have used (4.6).
To prove (4.13) it suffices now to show that

$$\biggl\| \Lambda_+^N \biggl(-\frac{\alpha Z}{|\mathbf{x}_N|} + \sum_{n=1}^{N-1} \frac{\alpha}{|\mathbf{x}_n - \mathbf{x}_N|} \biggr) \Lambda_+^N \Psi_j \biggr\| \underset{j\to\infty}{\longrightarrow} 0. \tag{4.16}$$

Let

$$\eta_1 \in C_0^\infty(\mathbb{R}^3), \quad \eta_1(\mathbf{x}) \equiv \begin{cases} 1, & \mathbf{x} \in B(1/2), \\ 0, & \mathbf{x} \in \mathbb{R}^3 \setminus B(3/4), \end{cases} \qquad \eta_j(\mathbf{x}) := \eta_1(\mathbf{x}/R_j), \quad j \in \mathbb{N}.$$

We estimate now the term in (4.16) corresponding to the interaction with the nucleus.

$$\begin{aligned}\Bigl\| \Lambda_+^N \frac{\alpha Z}{|\mathbf{x}_N|} \Lambda_+^N \Psi_j \Bigr\| \leqslant \alpha Z \biggl(&\Bigl\| \frac{\eta_j(\mathbf{x}_N)}{|\mathbf{x}_N|} (\Lambda_+ \psi_j)(\mathbf{x}_N) \Bigr\| \\ &+ \Bigl\| \frac{(1 - \eta_j(\mathbf{x}_N))}{|\mathbf{x}_N|} (\Lambda_+ \psi_j)(\mathbf{x}_N) \Bigr\| \biggr).\end{aligned} \tag{4.17}$$

For the first term in (4.17) the Hardy inequality and the commutativity of Λ_+ with ∇ imply

$$\Bigl\| \frac{\eta_j(\mathbf{x}_N)}{|\mathbf{x}_N|} (\Lambda_+ \psi_j)(\mathbf{x}_N) \Bigr\| \leqslant 2\|\nabla \eta_j\|_{L_\infty(\mathbb{R}^3)} \|\Lambda_+ \psi_j\| + 2\|\Lambda_+ \nabla \psi_j\|_{L_2(B(3R_j/4))}. \tag{4.18}$$

The first term in (4.18) decays as $R_j \to \infty$, since it is bounded by $2\|\nabla \eta_1\|_{L_\infty(\mathbb{R}^3)} R_j^{-1}$. Applying Lemma 2 to the second term on the r. h. s. of (4.18),

we arrive at

$$
\begin{aligned}
\|\Lambda_+\nabla\psi_j\|_{L_2(B(3R_j/4))} &\leqslant \Big(\frac{4\pi}{3}\Big(\frac{3R_j}{4}\Big)^3\Big)^{1/2}\|\Lambda_+\nabla\psi_j\|_{L_\infty(B(3R_j/4))} \\
&\leqslant \Big(\frac{4\pi}{3}\Big(\frac{3R_j}{4}\Big)^3\Big)^{1/2} G(R_j/4)\Big(\frac{4\pi}{3}(2R_j)^3\Big)^{1/2}\|\nabla\psi_j\|_{L_2(\mathbb{R}^3)}.
\end{aligned}
\tag{4.19}
$$

The last factor in (4.19) is bounded uniformly in j. The function G and consequently the r. h. s. of (4.19) decays exponentially as $R_j \to \infty$. We can estimate the second term in (4.17) by $2\alpha Z/R_j$. Hence the r. h. s. of (4.17) tends to 0 as $R_j \to \infty$.

Let us turn to the interaction between the N^{th} and the n^{th} electrons. We have

$$
\begin{aligned}
\Big\|\Lambda_+^N \frac{\alpha}{|\mathbf{x}_n-\mathbf{x}_N|}\Lambda_+^N\Psi_j\Big\| &\leqslant \Big\|\frac{\alpha\rho_{\varphi_j}(\mathbf{x}_n)}{|\mathbf{x}_n-\mathbf{x}_N|}(\Lambda_+\psi_j)(\mathbf{x}_N)\Big\|_{\{|\mathbf{x}_n|\geqslant R_j/4\}} \\
&+ \Big\|\frac{\alpha\rho_{\varphi_j}(\mathbf{x}_n)}{|\mathbf{x}_n-\mathbf{x}_N|}\eta_j(\mathbf{x}_N)(\Lambda_+\psi_j)(\mathbf{x}_N)\Big\|_{\{|\mathbf{x}_n|<R_j/4\}} \\
&+ \Big\|\frac{\alpha\rho_{\varphi_j}(\mathbf{x}_n)}{|\mathbf{x}_n-\mathbf{x}_N|}\big(1-\eta_j(\mathbf{x}_N)\big)(\Lambda_+\psi_j)(\mathbf{x}_N)\Big\|_{\{|\mathbf{x}_n|<R_j/4\}},
\end{aligned}
\tag{4.20}
$$

where

$$
\rho_{\varphi_j}(\mathbf{x}_n) = \int\limits_{\mathbb{R}^{3(N-2)}} \big|\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})\big|^2 d\mathbf{x}_1\cdots d\mathbf{x}_{n-1}d\mathbf{x}_{n+1}\cdots d\mathbf{x}_{N-1} \tag{4.21}
$$

if $N>2$, and $\rho_{\varphi_j} = |\varphi_j|^2$ if $N=2$; $\|\rho_{\varphi_j}\|_{L_2(\mathbb{R}^3)} = 1$. By the Hardy inequality the fist term in (4.20) can be estimated as

$$
\Big\|\frac{\alpha\rho_{\varphi_j}(\mathbf{x}_n)}{|\mathbf{x}_n-\mathbf{x}_N|}(\Lambda_+\psi_j)(\mathbf{x}_N)\Big\|_{\{|\mathbf{x}_n|\geqslant R_j/4\}} \leqslant 2\alpha\|\nabla\psi_j\|\|\rho_{\varphi_j}\|_{L_2(\mathbb{R}^3\setminus B(R_j/4))}. \tag{4.22}
$$

For the second term in (4.20) analogously to (4.18) and (4.19) we have

$$
\begin{aligned}
\Big\|\frac{\alpha\rho_{\varphi_j}(\mathbf{x}_n)}{|\mathbf{x}_n-\mathbf{x}_N|}\eta_j(\mathbf{x}_N)(\Lambda_+\psi_j)(\mathbf{x}_N)\Big\|_{\{|\mathbf{x}_n|<R_j/4\}} &\leqslant 2\alpha\|\nabla\eta_1\|_{L_\infty(\mathbb{R}^3)}R_j^{-1} \\
+2\alpha\Big(\frac{4\pi}{3}\Big(\frac{3R_j}{4}\Big)^3\Big)^{1/2} G(R_j/4)&\Big(\frac{4\pi}{3}(2R_j)^3\Big)^{1/2}\|\nabla\psi_j\|_{L_2(\mathbb{R}^3)}.
\end{aligned}
\tag{4.23}
$$

Finally, the last term on the r. h. s. of (4.20) can be estimated by $4\alpha/R_j$, since on the domain of integration $|\mathbf{x}_n - \mathbf{x}_N| > R_j/4$.

Combining these estimates, we arrive at (4.13). Lemma 8 is proved. •

Our next goal is to prove that the functions $\{\Psi_j\}_{j=1}^\infty$ can be antisymmetrized without violation of the condition (4.2) at least for j big enough.

Let

$$(T_{kN}\Psi_j)(\mathbf{x}_1,\dots,\mathbf{x}_N) := \varphi(\mathbf{x}_1,\dots,\mathbf{x}_{k-1},\mathbf{x}_N,\mathbf{x}_{k+1},\dots,\mathbf{x}_{N-1})\otimes\psi_j(\mathbf{x}_k),$$
$$k=1,\dots,N-1,\quad T_{NN}\Psi_j := -\Psi_j,\quad j\in\mathbb{N}. \tag{4.24}$$

The operator T_{kN} permutes the k^{th} and the N^{th} electrons. The functions $P_A\Psi_j$ are given by

$$(P_A\Psi_j)(\mathbf{x}_1,\dots,\mathbf{x}_N) = \frac{-1}{\sqrt{N}}\sum_{k=1}^{N-1} T_{kN}\Lambda_+^N\Psi_j(\mathbf{x}_1,\dots,\mathbf{x}_N),\quad j\in\mathbb{N}. \tag{4.25}$$

For the norms of these functions we have

$$\begin{aligned}\|P_A\Psi_j\|^2 &= \frac{1}{N}\langle\sum_{k=1}^{N-1} T_{kN}\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N),\\ &\qquad\qquad \sum_{l=1}^{N-1} T_{lN}\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N)\rangle\\ &\geqslant 1-\frac{N-1}{2}\big|\langle\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N),(\Lambda_+\psi_j)(\mathbf{x}_1)\varphi_j(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\big|,\end{aligned} \tag{4.26}$$

where the scalar products are taken in $\overset{N}{\underset{n=1}{\otimes}} L_2(\mathbb{R}^3,\mathbb{C}^4)$. To estimate the inner product on the r. h. s. of (4.26), we write

$$\begin{aligned}&\big|\langle\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N),(\Lambda_+\psi_j)(\mathbf{x}_1)\varphi_j(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\big|\\ &\leqslant \big|\langle\big(1-I_{B(R_j/2)}(\mathbf{x}_1)\big)\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N),\\ &\qquad\qquad (\Lambda_+\psi_j)(\mathbf{x}_1)\varphi_j(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\big|\\ &+\Big|\langle\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_j)(\mathbf{x}_N),I_{B(R_j/2)}(\mathbf{x}_1)(\Lambda_+\psi_j)(\mathbf{x}_1)\varphi_j(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\Big|.\end{aligned} \tag{4.27}$$

The first term on the r. h. s. of (4.27) tends to zero since $\Big\|\big(1-I_{B(R_j/2)}(\mathbf{x}_1)\big)\varphi_j(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})\Big\|_{L_2(\mathbb{R}^{N-1},\mathbb{C}^{4(N-1)})}$ does. The second one also vanishes, because by Lemma 2

$$\Big\|I_{B(R_j/2)}(\mathbf{x}_1)(\Lambda_+\psi_j)(\mathbf{x}_1)\Big\| \underset{R_j\to\infty}{\longrightarrow} 0.$$

This completes the proof of (4.1).

5 Proof of Theorem 1: "Hard Part"

We shall prove that

$$\inf\ \sigma_{\mathrm{ess}}(\mathcal{H}_N) \geqslant E_{N-1}+1. \tag{5.1}$$

Together with (4.1) this gives (2.5).

5.1 Partition of Unity

For a function $\chi \in C^\infty\big(\mathbb{R}^3, [0,1]\big)$ with $\chi|_{B(1)} \equiv 0$ and $\chi|_{\mathbb{R}^3\setminus B(2)} \equiv 1$, let

$$\tilde{\chi}_a := \chi(\mathbf{x}_a), \quad a = 1 \dots N, \quad \tilde{\chi}_0 := \prod_{a=1}^{N} (1 - \tilde{\chi}_a).$$

Let

$$\varphi(\mathbf{x}) := \sum_{a=0}^{N} \tilde{\chi}_a^2(\mathbf{x}).$$

Obviously, there exists a constant $\delta > 0$ such that for any $\mathbf{x} \in \mathbb{R}^{3N}$ we have $\delta < \varphi(\mathbf{x}) < \delta^{-1}$. For $R > 0$ we define a partition of unity

$$\chi_a(\mathbf{x}) := \frac{\tilde{\chi}_a(\mathbf{x}/R)}{\sqrt{\varphi(\mathbf{x}/R)}}, \quad \mathbf{x} \in \mathbb{R}^{3N}, \quad a = 0, \dots, N. \tag{5.2}$$

It is clear that the partition (5.2) satisfies all the hypotheses (3.27) of Lemma 6. Moreover, for $a \neq 0$ the functions χ_a are symmetric under all permutations of the electrons which do not include the a^{th} one. We also note that the derivatives of χ_a decay as R tends to infinity:

$$\|\nabla \chi_a\|_\infty \leqslant CR^{-1}, \quad \|\partial^2 \chi_a\|_\infty \leqslant CR^{-2}, \quad a = 0, \dots, N. \tag{5.3}$$

5.2 Estimates Outside the Compact Region

For $\varepsilon > 0$ we choose $R = R(\varepsilon)$ big enough so that the following conditions hold:
(i)

$$\widetilde{C}_{N,Z} \sum_{a \in \mathcal{A}} \big(\|\nabla \chi_a\|_{L_\infty(\mathbb{R}^{3N})} + \|\partial^2 \chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)\big(1 + \|\nabla \chi_a\|_{L_\infty(\mathbb{R}^{3N})}\big)^2 < \varepsilon, \tag{5.4}$$

where $\widetilde{C}_{N,Z}$ is the constant in (3.28),
(ii)

$$\frac{\alpha Z}{R} < \varepsilon(1 - \alpha Z), \tag{5.5}$$

(iii) For any $\psi \in \Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ and $a = 1, \dots, N$

$$\begin{aligned} \Big| \big\langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|}\Big) [\Lambda_+^N, \chi_a]\psi, \Lambda_+^N \chi_a \psi \big\rangle \\ + \big\langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|}\Big) \chi_a \psi, [\Lambda_+^N, \chi_a]\psi \big\rangle \Big| < \frac{\varepsilon}{N} \langle \mathcal{H}_N \psi, \psi \rangle. \end{aligned} \tag{5.6}$$

The possibility to fulfil (5.6) choosing R big enough follows from the Kato inequality and Lemmata 3, 4, and 5.

We now estimate from below the quadratic form of $\mathcal{H}_N$ on a function ψ from $\Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$. Recall that $\Lambda_+^N \bigwedge_{n=1}^{N} H^{1/2}(\mathbb{R}^3, \mathbb{C}^4)$ is the form domain of $\mathcal{H}_N$. By Lemma 6 and (5.4)

$$\langle \mathcal{H}_N \psi, \psi \rangle \geqslant \sum_{a=0}^{N} \langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle - \varepsilon \langle \mathcal{H}_N \psi, \psi \rangle. \tag{5.7}$$

For $a = 1, \ldots, N$ we have

$$\langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle = \langle \Big(\mathcal{H}_{N-1} + D_a - \frac{\alpha Z}{|\mathbf{x}_a|} + \sum_{k \neq a} \frac{\alpha}{|\mathbf{x}_a - \mathbf{x}_k|} \Big) \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle, \tag{5.8}$$

where $\mathcal{H}_{N-1}$ acts on the coordinates of all electrons except the a^{th} one. The inequalities $\mathcal{H}_{N-1} \geqslant E_{N-1}$, $\Lambda_+^N D_a \Lambda_+^N \geqslant 1$, and $\sum_{k \neq a} \frac{\alpha}{|\mathbf{x}_a - \mathbf{x}_k|} > 0$ for $a = 1, \ldots, N$ imply

$$\begin{aligned} \langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle &\geqslant \langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|} \Big) \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle \\ = \langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|} \Big) \chi_a \psi, \chi_a \psi \rangle &+ \langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|} \Big) [\Lambda_+^N, \chi_a] \psi, \Lambda_+^N \chi_a \psi \rangle \\ &+ \langle \Big(E_{N-1} + 1 - \frac{\alpha Z}{|\mathbf{x}_a|} \Big) \chi_a \psi, [\Lambda_+^N, \chi_a] \psi \rangle. \end{aligned} \tag{5.9}$$

Since on supp χ_a we have $|\mathbf{x}_a| \geqslant R$, from the relations (5.5), (5.6), and (5.9) we conclude

$$\begin{aligned} \langle \mathcal{H}_N \Lambda_+^N \chi_a \psi, \Lambda_+^N \chi_a \psi \rangle \geqslant (E_{N-1} + 1) \langle \chi_a \psi, \chi_a \psi \rangle \\ - \frac{\varepsilon}{N} \langle \mathcal{H}_N \psi, \psi \rangle - \varepsilon (1 - \alpha Z) \|\psi\|^2, \quad a = 1, \ldots, N. \end{aligned} \tag{5.10}$$

Using (3.24), we arrive at

$$\langle \mathcal{H}_N \psi, \psi \rangle \geqslant \langle \sum_{n=1}^{N} \Big(D_n - \frac{\alpha Z}{|\mathbf{x}_n|} \Big) \psi, \psi \rangle \geqslant N(1 - \alpha Z) \|\psi\|^2. \tag{5.11}$$

Due to (5.7), (5.10), and (5.11)

$$(1 + 3\varepsilon) \langle \mathcal{H}_N \psi, \psi \rangle \geqslant (E_{N-1} + 1) \sum_{a=1}^{N} \langle \chi_a \psi, \chi_a \psi \rangle + \langle \mathcal{H}_N \Lambda_+^N \chi_0 \psi, \Lambda_+^N \chi_0 \psi \rangle. \tag{5.12}$$

5.3 Estimate Inside the Compact Region

Our next goal is to estimate from below the quadratic form of the operator $H_N\Lambda_+^N$ on the function $\chi_0\psi$ supported in $[-2R,2R]^{3N}$.

Lemma 9 *For $M>0$ let $W_M := \{\mathbf{p}\in\mathbb{R}^{3N}\,\big|\,|p_i|\leqslant M, i=1,\dots,3N\}$, $\widetilde{W}_M := \mathbb{R}^{3N}\setminus W_M$. There exists a finite set Q_M of functions in $L_2(\mathbb{R}^{3N})$ such that for any function $f\in L_2(\mathbb{R}^{3N})$ with $\mathrm{supp} f\subset[-2R,2R]^{3N}$, $f\perp Q_M$ holds*

$$\|\hat f\|_{L_2(\widetilde{W}_M)} \geqslant \frac{1}{2}\|\hat f\|_{L_2(\mathbb{R}^{3N})}. \tag{5.13}$$

The proof of Lemma 9 is analogous to the proof of Theorem 7 in [25] and will be given in the Appendix C for convenience.

It follows from (3.25) that for any $M>0$

$$\begin{aligned}\langle\mathcal{H}_N\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle &= \langle\Big(\sum_{n=1}^N\Big(D_n-\frac{\alpha Z}{|\mathbf{x}_n|}\Big)+\sum_{n<j}\frac{\alpha}{|\mathbf{x}_n-\mathbf{x}_j|}\Big)\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle\\ &\geqslant \frac{Z_c-Z}{Z_c}\langle\sum_{n=1}^N D_n I_{\widetilde{W}_M}\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle.\end{aligned} \tag{5.14}$$

Here $I_{\widetilde{W}_M}$ is the operator of multiplication by the characteristic function of $\widetilde{W}_M$ in momentum space.

We choose

$$M := \sqrt{\Big(\frac{8Z_c(E_{N-1}+1)}{Z_c-Z}\Big)^2-1} \tag{5.15}$$

and assume henceforth that $f:=\chi_0\psi$ is orthogonal to the set Q_M defined in Lemma 9. Since in momentum space the operator D acts on functions from $\Lambda_+L_2(\mathbb{R}^3,\mathbb{C}^4)$ as multiplication by $\sqrt{|\mathbf{k}|^2+1}$, we have

$$\langle\sum_{n=1}^N D_n I_{\widetilde{W}_M}\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle \geqslant \sqrt{M^2+1}\|I_{\widetilde{W}_M}\Lambda_+^N\chi_0\psi\|^2. \tag{5.16}$$

Inequalities (5.14) and (5.16) imply

$$\begin{aligned}&\langle\mathcal{H}_N\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle \geqslant \frac{Z_c-Z}{Z_c}\sqrt{M^2+1}\|I_{\widetilde{W}_M}\Lambda_+^N\chi_0\psi\|^2\\ &\geqslant \frac{Z_c-Z}{Z_c}\sqrt{M^2+1}\Big(\|I_{\widetilde{W}_M}\chi_0\psi\| - \big\|I_{\widetilde{W}_M}[\Lambda_+^N,\chi_0]\psi\big\|\Big)^2\\ &\geqslant \frac{Z_c-Z}{Z_c}\sqrt{M^2+1}\Big(\frac{1}{2}\|I_{\widetilde{W}_M}\chi_0\psi\|^2 - \big\|I_{\widetilde{W}_M}[\Lambda_+^N,\chi_0]\psi\big\|^2\Big)\\ &\geqslant 4(E_{N-1}+1)\|I_{\widetilde{W}_M}\chi_0\psi\|^2\\ &\qquad - 8(E_{N-1}+1)\big\|[\Lambda_+^N,\chi_0]\big\|^2_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})\to L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\|\psi\|^2.\end{aligned} \tag{5.17}$$

In the last step we used our choice of M (see (5.15)). Since Λ_+ is a bounded operator in $L_2(\mathbb{R}^3,\mathbb{C}^4)$, and

$$\big\|[\chi_0,\Lambda_+^N]\big\|_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})\to L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\leqslant C\big(\|\nabla\chi_0\|_\infty+\|\partial^2\chi_0\|_\infty\big)$$

by Lemma 1 and the relation (3.22), we can choose R big enough, so that

$$8|E_{N-1}+1|\big\|[\Lambda_+^N,\chi_0]\big\|^2_{L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})\to L_2(\mathbb{R}^{3N},\mathbb{C}^{4^N})}\leqslant\varepsilon. \tag{5.18}$$

For the first term on the r. h. s. of (5.17) Lemma 9 implies

$$4\|I_{\widetilde{W}_M}\chi_0\psi\|^2\geqslant\|\chi_0\psi\|^2. \tag{5.19}$$

As a consequence of (5.17) — (5.19), we have

$$\langle\mathcal{H}_N\Lambda_+^N\chi_0\psi,\Lambda_+^N\chi_0\psi\rangle\geqslant(E_{N-1}+1)\|\chi_0\psi\|^2-\varepsilon\|\psi\|^2. \tag{5.20}$$

5.4 Completion of the Proof

By (5.12) and (5.20)

$$(1+3\varepsilon)\langle\mathcal{H}_N\psi,\psi\rangle\geqslant(E_{N-1}+1)\sum_{a=0}^{N}\langle\chi_a\psi,\chi_a\psi\rangle-\varepsilon\|\psi\|^2=(E_{N-1}+1-\varepsilon)\|\psi\|^2 \tag{5.21}$$

for any $\varepsilon>0$ and any ψ in the form domain of $\mathcal{H}_N$ orthogonal to the finite set of functions (cardinality of this set depends on ε). This implies the discreteness of the spectrum of $\mathcal{H}_N$ below $E_{N-1}+1$ and thus (5.1).

6 Existence of Eigenvalues

1. To prove the infiniteness of the discrete spectrum of $\mathcal{H}_N$ it suffices to construct for a given $Q\in\mathbb{N}$ a Q–dimensional subspace $\mathcal{M}$ such that for any $\Psi\in\mathcal{M}$ we have $\langle\mathcal{H}_N\Psi,\Psi\rangle<(E_{N-1}+1)\|\Psi\|^2$.

Using induction on N and the well–known existence of the ground state of $\mathcal{H}_1$, we can assume that $\mathcal{H}_{N-1}$ has a ground state ϕ. Let $\widetilde{\psi}\in C_0^\infty(\mathbb{R}^3,\mathbb{C}^4)$ be a function with supp $\widetilde{\psi}\subset B(N-\frac{1}{5})\setminus B(N-\frac{2}{5})$, whose 3^{rd} and 4^{th} components are identical to zero. Let $\|\widetilde{\psi}\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}=1$. Let

$$\psi_m(\mathbf{y}):=R_m^{-3/2}\widetilde{\psi}\Big(\frac{\mathbf{y}}{R_m}\Big),\quad R_m:=2^mR,\quad m=1,\dots Q. \tag{6.1}$$

The parameter R will be chosen later. Note that $\Lambda_+\psi_m\neq0$ for large R due to (3.1) and the choice of the components of $\widetilde{\psi}$.

We consider the quadratic form of $\mathcal{H}_N$ on linear combinations of the form

$$\sum_{m=1}^{Q} c_m \sum_{k=1}^{N} T_{kN}(\phi \otimes \Lambda_+ \psi_m). \tag{6.2}$$

Here T_{kN} for $k < N$ is the operator permuting the k^{th} and the N^{th} electrons, $T_{NN} := -1$. In the tensor product $\phi \otimes \Lambda_+ \psi_m$ the function ϕ is assumed to depend on $\mathbf{x}_1, \ldots, \mathbf{x}_{N-1}$, and ψ_m depends on $\mathbf{x}_N$. The functions (6.2) are antisymmetric in all variables.

It suffices to show that on the functions (6.2) the quadratic form of

$$\widetilde{\mathcal{H}}_N := \mathcal{H}_N - E_{N-1} - 1$$

is negative for any choice of the coefficients $\{c_m\}_{m=1}^{Q}$.

Using the permutation symmetry of ϕ and $\widetilde{\mathcal{H}}_N$, we can write

$$\begin{aligned}
&\langle \widetilde{\mathcal{H}}_N \sum_{m=1}^{Q} c_m \sum_{k=1}^{N} T_{kN}(\phi \otimes \Lambda_+ \psi_m), \sum_{n=1}^{Q} c_n \sum_{l=1}^{N} T_{lN}(\phi \otimes \Lambda_+ \psi_n)\rangle \\
&= \sum_{m=1}^{Q} |c_m|^2 \sum_{k,l=1}^{N} \langle \widetilde{\mathcal{H}}_N T_{kN}(\phi \otimes \Lambda_+ \psi_m), T_{lN}(\phi \otimes \Lambda_+ \psi_m)\rangle \\
&+2 \sum_{n<m} c_m \overline{c_n} \sum_{k,l=1}^{N} \langle \widetilde{\mathcal{H}}_N T_{kN}(\phi \otimes \Lambda_+ \psi_m), T_{lN}(\phi \otimes \Lambda_+ \psi_n)\rangle \\
&\leqslant \sum_{m=1}^{Q} |c_m|^2 \Big\{ N \langle \widetilde{\mathcal{H}}_N (\phi \otimes \Lambda_+ \psi_m), \phi \otimes \Lambda_+ \psi_m \rangle \\
&+ \frac{N(N-1)}{2} \sum_{n=1}^{Q} \big| \langle \widetilde{\mathcal{H}}_N (\phi \otimes \Lambda_+ \psi_m), T_{1N}(\phi \otimes \Lambda_+ \psi_n)\rangle \big| \\
&+ N \sum_{n \neq m}^{Q} \big| \langle \widetilde{\mathcal{H}}_N (\phi \otimes \Lambda_+ \psi_m), \phi \otimes \Lambda_+ \psi_n \rangle \big| \Big\}.
\end{aligned} \tag{6.3}$$

Our strategy is to show that the first term on the r. h. s. of (6.3) is negative and of the order R^{-1} as $R \to \infty$, whereas the other terms decay more rapidly.

2. For the first term on the r. h. s. of (6.3) we have

$$\begin{aligned}
&\langle \widetilde{\mathcal{H}}_N (\phi \otimes \Lambda_+ \psi_m), \phi \otimes \Lambda_+ \psi_m \rangle \\
&= \langle (D-1)\Lambda_+ \psi_m, \Lambda_+ \psi_m \rangle - \langle \frac{\alpha Z}{|\mathbf{x}|} \Lambda_+ \psi_m, \Lambda_+ \psi_m \rangle \\
&+ \sum_{i<N} \langle \frac{\alpha}{|\mathbf{x}_i - \mathbf{x}_N|} \rho_\phi(\mathbf{x}_i)(\Lambda_+ \psi_m)(\mathbf{x}_N), \rho_\phi(\mathbf{x}_i)(\Lambda_+ \psi_m)(\mathbf{x}_N)\rangle
\end{aligned} \tag{6.4}$$

with ρ_ϕ defined in (4.21).

We start with the lower bound on the first term on the r. h. s. of (6.4). Recall that ψ_1 has the last two components equal to zero, thus relations (6.1), (2.2), and (3.1) imply

$$\begin{aligned}
&\langle (D\Lambda_+ - \Lambda_+)\psi_m, \psi_m\rangle \\
&\quad =\langle \Big(\frac{1}{2} + \frac{\sqrt{|\mathbf{q}|^2 + R_m^2}}{2R_m} - \frac{1}{2} - \frac{R_m}{2\sqrt{|\mathbf{q}|^2 + R_m^2}}\Big)\hat{\psi}_1(\mathbf{q}), \hat{\psi}_1(\mathbf{q})\rangle \\
&\quad = \langle \frac{|\mathbf{q}|^2}{2R_m\sqrt{|\mathbf{q}|^2 + R_m^2}}\hat{\psi}_1(\mathbf{q}), \hat{\psi}_1(\mathbf{q})\rangle \leqslant \frac{1}{2R_m^2}\big\||\mathbf{q}|\hat{\psi}_1(\mathbf{q})\big\|^2.
\end{aligned} \tag{6.5}$$

Here $\mathbf{q}$ is the momentum dual to $\mathbf{y}$ in (6.1). The norm in (6.5) is finite, since $\tilde{\psi}_1 \in C_0^\infty(\mathbb{R}^3, \mathbb{C}^4)$.

To estimate the interaction of an electron with the nucleus we choose

$$\delta := \frac{1}{10N - 8}. \tag{6.6}$$

Obviously,

$$\begin{aligned}
&-\langle \frac{\alpha Z}{|\mathbf{x}|}\Lambda_+\psi_m, \Lambda_+\psi_m\rangle \\
&= -\langle \frac{\alpha Z}{|\mathbf{x}|} I_{B(ZR_m)}\Lambda_+\psi_m, \Lambda_+\psi_m\rangle - \langle \frac{\alpha Z}{|\mathbf{x}|}(1 - I_{B(ZR_m)})\Lambda_+\psi_m, \Lambda_+\psi_m\rangle \\
&\leqslant -\frac{\alpha}{R_m}\Big(\|\Lambda_+\psi_m\| - \big\|(1 - I_{B(ZR_m)})\Lambda_+\psi_m\big\|\Big)^2 + \frac{\alpha}{R_m}\big\|(1 - I_{B(ZR_m)})\Lambda_+\psi_m\big\|^2 \\
&\leqslant -\frac{(1-\delta)\alpha}{R_m}\|\Lambda_+\psi_m\|^2 + \frac{(2 + \delta^{-1})\alpha}{R_m}\big\|(1 - I_{B(ZR_m)})\Lambda_+\psi_m\big\|^2.
\end{aligned} \tag{6.7}$$

Lemma 2 implies

$$\begin{aligned}
&\big\|(1 - I_{B(ZR_m)})\Lambda_+\psi_m\big\|^2 \\
&\qquad \leqslant \int_{ZR_m}^{\infty} 4\pi r^2 G^2\Big(r - \big(N - \frac{1}{5}\big)R_m\Big)\frac{4\pi}{3}\Big(N - \frac{1}{5}\Big)^3 R_m^3\|\psi_m\|^2 dr \\
&\qquad \leqslant \frac{16\pi^2}{3}\Big(N - \frac{1}{5}\Big)^3 R_m^3 \int_{ZR_m}^{\infty} G^2\Big(r - \big(N - \frac{1}{5}\big)R_m\Big) r^2 dr,
\end{aligned}$$

which is a function decaying faster than any power of R_m.

Now we turn to estimating the electron–electron interaction. We split the

corresponding quadratic form into three integrals:

$$
\begin{aligned}
&\langle \frac{\alpha}{|\mathbf{x}_i - \mathbf{x}_N|} \rho_\phi(\mathbf{x}_i)(\Lambda_+\psi_m)(\mathbf{x}_N), \rho_\phi(\mathbf{x}_i)(\Lambda_+\psi_m)(\mathbf{x}_N)\rangle \\
&= \alpha\Big(\iint\limits_{|\mathbf{x}|\geqslant R_m/5} + \iint\limits_{\substack{|\mathbf{x}|<R_m/5 \\ |\mathbf{y}|<(N-3/5)R_m}} + \iint\limits_{\substack{|\mathbf{x}|<R_m/5 \\ |\mathbf{y}|\geqslant(N-3/5)R_m}} \Big) \frac{\big|\rho_\phi(\mathbf{x})\big|^2}{|\mathbf{x}-\mathbf{y}|} \big|(\Lambda_+\psi_m)(\mathbf{y})\big|^2 d\mathbf{x}d\mathbf{y} \qquad (6.8) \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad =: I_1 + I_2 + I_3.
\end{aligned}
$$

From the Kato inequality (see [14], inequality V.5.33; see also [9])

$$
\int\limits_{\mathbb{R}^3} |\mathbf{x}|^{-1}\big|u(\mathbf{x})\big|^2 d\mathbf{x} \leqslant \frac{\pi}{2} \int\limits_{\mathbb{R}^3} |\mathbf{k}|\big|\hat{u}(\mathbf{k})\big|^2 d\mathbf{k}, \quad \forall u \in H^{1/2}(\mathbb{R}^3) \tag{6.9}
$$

it follows that

$$
I_1 \leqslant \frac{\pi\alpha}{2R_m} \|\rho_\phi\|^2_{L_2(\mathbb{R}^3\setminus B(R_m/5))} \big\||\mathbf{q}|^{1/2}\hat{\psi}_1(\mathbf{q})\big\|^2_{L_2(\mathbb{R}^3)}. \tag{6.10}
$$

Using Lemma 2, we arrive at

$$
I_2 \leqslant \frac{4\pi\alpha}{3}\Big(N - \frac{1}{5}\Big)^3 R_m^3 G^2\Big(\frac{R_m}{5}\Big)\|\Lambda_+\psi_m\|^2 \int\limits_{|\mathbf{x}|<\frac{R_m}{5}} \big|\rho_\phi(\mathbf{x})\big|^2 \int\limits_{|\mathbf{y}|<(N-\frac{3}{5})R_m} \frac{1}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y}d\mathbf{x}. \tag{6.11}
$$

Here

$$
\int\limits_{|\mathbf{y}|<(N-3/5)R_m} \frac{1}{|\mathbf{x}-\mathbf{y}|} d\mathbf{y} \leqslant \int\limits_{|\mathbf{y}|<(N-3/5)R_m} \frac{1}{|\mathbf{y}|} d\mathbf{y} \leqslant 2\pi\Big(N - \frac{3}{5}\Big)^2 R_m^2.
$$

Obviously, the r. h. s.'s of (6.10) and (6.11) decay faster than R_m^{-1}. Finally, for I_3 we have

$$
I_3 \leqslant \frac{\alpha}{\big(N - \frac{4}{5}\big)R_m} \|\Lambda_+\psi_m\|^2. \tag{6.12}
$$

Combining (6.4) — (6.12), for large R we get

$$
\begin{aligned}
&\langle \widetilde{\mathcal{H}}_N(\phi\otimes\Lambda_+\psi_m), \phi\otimes\Lambda_+\psi_m\rangle \\
&\qquad\qquad \leqslant \alpha\bigg(\frac{N-1}{\big(N-\frac{4}{5}\big)} - 1 + \delta\bigg)\|\Lambda_+\psi_m\|^2 R_m^{-1} + o(R^{-1}).
\end{aligned} \tag{6.13}
$$

The coefficient at R_m^{-1} is negative due to (6.6).

3. Let us prove now that the second term on the r. h. s. of (6.3) decays faster than R^{-1}.

$$\begin{aligned}
&\langle\widetilde{\mathcal{H}}_N(\phi\otimes\Lambda_+\psi_m), T_{1N}(\phi\otimes\Lambda_+\psi_n)\rangle\\
&\quad=\langle\Big((\mathcal{H}_{N-1}-E_{N-1})+(D_N-1)-\frac{\alpha Z}{|\mathbf{x}_N|}+\sum_{j=1}^{N-1}\frac{\alpha}{|\mathbf{x}_j-\mathbf{x}_N|}\Big)\\
&\qquad\quad\times\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_m)(\mathbf{x}_N),(\Lambda_+\psi_n)(\mathbf{x}_1)\phi(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle \qquad (6.14)\\
&\quad=\langle\Big((D_N-1)-\frac{\alpha Z}{|\mathbf{x}_N|}+\sum_{j=1}^{N-1}\frac{\alpha}{|\mathbf{x}_j-\mathbf{x}_N|}\Big)\\
&\qquad\quad\times\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_m)(\mathbf{x}_N),(\Lambda_+\psi_n)(\mathbf{x}_1)\phi(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle,
\end{aligned}$$

where $\mathcal{H}_{N-1}$ acts on the first $N-1$ electrons.

We introduce a cut–off function

$$\chi\in C_0^\infty(\mathbb{R}^3),\quad \chi(\mathbf{x})=\begin{cases}1, & |\mathbf{x}|\leqslant 1/4,\\ 0, & |\mathbf{x}|\geqslant 1/2,\end{cases}\quad \chi_n(\mathbf{x}):=\chi\Big(\frac{\mathbf{x}}{R_n}\Big). \qquad (6.15)$$

One has

$$\begin{aligned}
&\Big|\langle\Big((D_N-1)-\frac{\alpha Z}{|\mathbf{x}_N|}+\sum_{j=1}^{N-1}\frac{\alpha}{|\mathbf{x}_j-\mathbf{x}_N|}\Big)\\
&\qquad\times\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})(\Lambda_+\psi_m)(\mathbf{x}_N),(\Lambda_+\psi_n)(\mathbf{x}_1)\phi(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\Big|\\
&\leqslant\Big|\langle\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})\Big((D_N-1)-\frac{\alpha Z}{|\mathbf{x}_N|}+\sum_{j=1}^{N-1}\frac{\alpha}{|\mathbf{x}_j-\mathbf{x}_N|}\Big)\\
&\qquad\times(\Lambda_+\psi_m)(\mathbf{x}_N),\chi_n(\mathbf{x}_1)(\Lambda_+\psi_n)(\mathbf{x}_1)\phi(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\Big|\\
&+\Big|\langle\big(1-\chi_n(\mathbf{x}_1)\big)\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})\Big((D_N-1)-\frac{\alpha Z}{|\mathbf{x}_N|}+\sum_{j=1}^{N-1}\frac{\alpha}{|\mathbf{x}_j-\mathbf{x}_N|}\Big)\\
&\qquad\times(\Lambda_+\psi_m)(\mathbf{x}_N),(\Lambda_+\psi_n)(\mathbf{x}_1)\phi(\mathbf{x}_2,\dots,\mathbf{x}_N)\rangle\Big|\\
&\leqslant\Big(\big\|(D-1)\Lambda_+\psi_m\big\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}+2\alpha(Z+N-1)\|\nabla\psi_m\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}\Big)\\
&\times\Big(\|\chi_n\Lambda_+\psi_n\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)}+\Big\|\big(1-\chi_n(\mathbf{x}_1)\big)\phi(\mathbf{x}_1,\dots,\mathbf{x}_{N-1})\Big\|_{L_2(\mathbb{R}^{3(N-1)},\mathbb{C}^{4^{(N-1)}})}\Big),
\end{aligned} \qquad (6.16)$$

where for the electrostatic terms we have used the Hardy inequality, the fact that Λ_+ commutes with the gradient and the equality $\|\Lambda_+\|_{L_2(\mathbb{R}^3,\mathbb{C}^4)\to L_2(\mathbb{R}^3,\mathbb{C}^4)}=1$.

Since only the first two components of ψ_m are nonzero, we calculate

$$
\begin{aligned}
&\big\|(D-1)\Lambda_+\psi_m\big\|^2\\
&= \langle(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta-1)(\boldsymbol{\alpha}\cdot\mathbf{p}+\beta-1)\frac{\sqrt{|\mathbf{p}|^2+1}+\boldsymbol{\alpha}\cdot\mathbf{p}+\beta}{2\sqrt{|\mathbf{p}|^2+1}}\hat{\psi}_m(\mathbf{p}),\hat{\psi}_m(\mathbf{p})\rangle\\
&= \langle|\mathbf{p}|^2\Big(\frac{1}{2}-\frac{1}{2\sqrt{|\mathbf{p}|^2+1}}\Big)\hat{\psi}_m(\mathbf{p}),\hat{\psi}_m(\mathbf{p})\rangle\\
&= \langle\frac{|\mathbf{q}|^2}{R_m^2}\Big(\frac{1}{2}-\frac{R_m}{2\sqrt{|\mathbf{q}|^2+R_m^2}}\Big)\hat{\tilde{\psi}}(\mathbf{q}),\hat{\tilde{\psi}}(\mathbf{q})\rangle \leqslant \frac{1}{2R_m^2}\big\||\mathbf{q}|\hat{\tilde{\psi}}(\mathbf{q})\big\|^2.
\end{aligned}
\tag{6.17}
$$

Thus the first factor on the r. h. s. of (6.16) decays as $\|\nabla\psi_m\|$, which is of order R^{-1}. The first term in the second factor of (6.16) is an exponentially decaying function of R due to Lemma 2 and the support properties of ψ_n and χ_n. The second one also goes to zero as $R\to\infty$. We conclude that the second term on the r. h. s. of (6.3) decays faster than R^{-1}.

4. We proceed to the estimate of the last term on the r. h. s. of (6.3). The key tool here is Lemma 2. We use the relation

$$
\begin{aligned}
&\langle\widetilde{\mathcal{H}}_N(\phi\otimes\Lambda_+\psi_m),\phi\otimes\Lambda_+\psi_n\rangle\\
&= \langle(D-1)\Lambda_+\psi_m,\Lambda_+\psi_n\rangle - \langle\frac{\alpha Z}{|\mathbf{x}|}\Lambda_+\psi_m,\Lambda_+\psi_n\rangle\\
&+\sum_{i<N}\langle\frac{\alpha}{|\mathbf{x}_i-\mathbf{x}_N|}\rho_\phi(\mathbf{x}_i)(\Lambda_+\psi_m)(\mathbf{x}_N),\rho_\phi(\mathbf{x}_i)(\Lambda_+\psi_n)(\mathbf{x}_N)\rangle.
\end{aligned}
\tag{6.18}
$$

For the kinetic energy term we have

$$
\begin{aligned}
\big|\langle(D\Lambda_+-\Lambda_+)\psi_m,\Lambda_+\psi_n\rangle\big| &= \big|\langle\Lambda_+\psi_m,(D-1)\psi_n\rangle\big|\\
&\leqslant \|\Lambda_+\psi_m\|_{L_2(\operatorname{supp}\psi_n)}\big\|(D-1)\psi_n\big\|.
\end{aligned}
\tag{6.19}
$$

Notice that the norm $\big\|(D-1)\psi_n\big\|$ is bounded uniformly in n and R.

Since

$$
\operatorname{supp}\psi_k\subset B\bigg(2^kR\Big(N-\frac{1}{5}\Big)\bigg)\setminus B\bigg(2^kR\Big(N-\frac{2}{5}\Big)\bigg),\quad k=1,\ldots,Q,
$$

Lemma 2 implies the exponential decay of $\|\Lambda_+\psi_m\|_{L_2(\operatorname{supp}\psi_n)}$, and hence of the r. h. s. of (6.19), in R.

Let B_{mn} be the ball with the radius $\frac{1}{2}(R_m+R_m)$ centered at the origin. For the interaction with the nucleus one has

$$
\begin{aligned}
&\langle-\frac{\alpha Z}{|\mathbf{x}_N|}\Lambda_+\psi_m,\Lambda_+\psi_n\rangle\\
&= \alpha Z\Big(\int_{B_{mn}}+\int_{\mathbb{R}^3\setminus B_{mn}}\Big)\frac{1}{|\mathbf{x}_N|}(\Lambda_+\psi_n)^*(\mathbf{x}_N)(\Lambda_+\psi_m)(\mathbf{x}_N)d\mathbf{x}_N.
\end{aligned}
\tag{6.20}
$$

Without loss of generality assume $n > m$. By Lemma 2

$$\|\Lambda_+\psi_n\|_{L_2(B_{mn})} \leqslant Ce^{-\delta R} \tag{6.21}$$

for some $C > 0$ and $\delta > 0$ independent of m and n.
By the Hardy inequality

$$\Big\|\frac{1}{|\mathbf{x}_N|}\Lambda_+\psi_m\Big\| \leqslant 2\|\nabla\Lambda_+\psi_m\| \leqslant C_1|R_m|^{-1}. \tag{6.22}$$

Together with (6.21) this implies

$$\Big|\int\limits_{B_{mn}} \frac{1}{|\mathbf{x}_N|}(\Lambda_+\psi_n)^*(\mathbf{x}_N)(\Lambda_+\psi_m)(\mathbf{x}_N)d\mathbf{x}_N\Big| \leqslant Ce^{-\delta R}. \tag{6.23}$$

Similarly, in $\mathbb{R}^3 \setminus B_{mn}$ the estimates (6.21), (6.22), and (6.23) hold if we replace everywhere $m \leftrightarrow n$ and B_{mn} by $\mathbb{R}^3 \setminus B_{mn}$.

It follows that

$$\Big|\langle\frac{\alpha Z}{|\mathbf{x}|}\Lambda_+\psi_m, \Lambda_+\psi_n\rangle\Big| \leqslant Ce^{-\delta R}. \tag{6.24}$$

The last term in (6.18), which describes the electron–electron interaction, can be estimated analogously to (6.20) — (6.24). Together with (6.19) and (6.24) this implies

$$\big|\langle\widetilde{\mathcal{H}}_N(\phi\otimes\Lambda_+\psi_m), \phi\otimes\Lambda_+\psi_n\rangle\big| \leqslant Ce^{-\delta R},$$

which completes the proof of Theorem 2.

A Some Properties of the Bessel Functions K_ν

The modified Bessel (McDonald) functions are related to the Hankel functions by the formula

$$K_\nu(z) = \frac{\pi}{2}e^{i\pi(\nu+1)/2}H_\nu^{(1)}(iz).$$

These functions are positive and decaying for $z \in (0,\infty)$. Their asymptotics are (see [8] 8.446, 8.447.3, 8.451.6)

$$\begin{aligned} &K_\nu(z) = \sqrt{\frac{\pi}{2z}}e^{-z}\Big(1 + O\Big(\frac{1}{z}\Big)\Big), \quad z \to +\infty; \\ &K_0(z) = -\log z\big(1 + o(1)\big), \quad K_1(z) = \frac{1}{z}\big(1 + o(1)\big), \quad z \to +0. \end{aligned} \tag{A.1}$$

The derivatives of these functions are (see [8] 8.486.12, 8.486.18)

$$K_0'(z) = -K_1(z), \quad K_1'(z) = -K_0(z) - \frac{1}{z}K_1(z), \quad z \in (0,\infty). \tag{A.2}$$

B Coordinate Representation for the Operator Λ_+

Lemma 10 *Let $f \in L_2(\mathbb{R}^3, \mathbb{C}^4) \cap C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ be a function in the coordinate representation. Then for $\Lambda_+ f$ formula* (3.2) *holds.*

Proof. We start with the operator $2\Lambda_+ - 1$, which is due to (3.1) the multiplication by the matrix function $\dfrac{\boldsymbol{\alpha} \cdot \mathbf{p} + \beta}{\sqrt{|\mathbf{p}|^2 + 1}}$ in the momentum space. It can be factorized as $A \cdot B$ with

$$A := (\boldsymbol{\alpha} \cdot \mathbf{p} + \beta)\big(|\mathbf{p}|^2 + 1\big), \quad B := \big(|\mathbf{p}|^2 + 1\big)^{-3/2}.$$

In coordinate representation $B : L_2(\mathbb{R}^3, \mathbb{C}^4) \to H^3(\mathbb{R}^3, \mathbb{C}^4)$ is a bounded integral operator. Its kernel is given by the convergent integral

$$\begin{aligned} B(\mathbf{x}, \mathbf{y}) &= \frac{1}{(2\pi)^3} \int\limits_{\mathbb{R}^3} \frac{e^{i\mathbf{p}\cdot(\mathbf{x}-\mathbf{y})}}{\big(|\mathbf{p}|^2 + 1\big)^{3/2}} d\mathbf{p} \\ &= \frac{1}{2\pi^2} \int\limits_0^\infty \frac{p \sin\big(p|\mathbf{x} - \mathbf{y}|\big)}{|\mathbf{x} - \mathbf{y}|(p^2 + 1)^{3/2}} dp = \frac{1}{2\pi^2} K_0\big(|\mathbf{x} - \mathbf{y}|\big). \end{aligned}$$

In configuration space A is the differential operator $(-i\boldsymbol{\alpha} \cdot \nabla + \beta)(-\Delta + 1)$ mapping $H^3(\mathbb{R}^3, \mathbb{C}^4)$ onto $L_2(\mathbb{R}^3, \mathbb{C}^4)$. Thus with the help of (A.2) for any $f \in L_2(\mathbb{R}^3, \mathbb{C}^4) \cap C_0^1(\mathbb{R}^3, \mathbb{C}^4)$ we get

$$\begin{aligned} \big((2\Lambda_+ - 1)f\big)(\mathbf{x}) &= (-i\boldsymbol{\alpha} \cdot \nabla + \beta)(-\Delta + 1) \frac{1}{2\pi^2} \int\limits_{\mathbb{R}^3} K_0\big(|\mathbf{x} - \mathbf{y}|\big) f(\mathbf{y}) d\mathbf{y} \\ &= (-i\boldsymbol{\alpha} \cdot \nabla + \beta) \frac{1}{2\pi^2} \int\limits_{\mathbb{R}^3} \frac{K_1\big(|\mathbf{x} - \mathbf{y}|\big)}{|\mathbf{x} - \mathbf{y}|} f(\mathbf{y}) d\mathbf{y} \qquad \text{(B.1)} \\ &= (-i\boldsymbol{\alpha} \cdot \nabla + \beta) \frac{1}{2\pi^2} \int\limits_{\mathbb{R}^3} \frac{K_1\big(|\mathbf{y}|\big)}{|\mathbf{y}|} f(\mathbf{x} - \mathbf{y}) d\mathbf{y}. \end{aligned}$$

The term with β defines a function from $L_2(\mathbb{R}^3, \mathbb{C}^4)$, because $|\cdot|^{-1} K_1\big(|\cdot|\big) \in L_1(\mathbb{R}^3)$. We rewrite the gradient term on the r. h. s. of (B.1) as

$$\begin{aligned} &-i\boldsymbol{\alpha} \cdot \nabla_{\mathbf{x}} \frac{1}{2\pi^2} \int\limits_{\mathbb{R}^3} \frac{K_1\big(|\mathbf{y}|\big)}{|\mathbf{y}|} f(\mathbf{x} - \mathbf{y}) d\mathbf{y} \\ &\quad = \frac{i}{2\pi^2} \Bigg(\int\limits_{\mathbb{R}^3 \setminus B(\varepsilon)} + \int\limits_{B(\varepsilon)} \Bigg) \frac{K_1\big(|\mathbf{y}|\big)}{|\mathbf{y}|} \boldsymbol{\alpha} \cdot \nabla_{\mathbf{y}} \big(f(\mathbf{x} - \mathbf{y})\big) d\mathbf{y}. \end{aligned} \qquad \text{(B.2)}$$

The second integral on the r. h. s. of (B.2) can be estimated as

$$\left|\frac{i}{2\pi^2}\int\limits_{B(\varepsilon)}\frac{K_1(|\mathbf{y}|)}{|\mathbf{y}|}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\big(f(\mathbf{x}-\mathbf{y})\big)d\mathbf{y}\right| \leqslant \frac{3}{2\pi^2}\|\nabla f\|_\infty\int\limits_{B(\varepsilon)}\frac{K_1(|\mathbf{y}|)}{|\mathbf{y}|}d\mathbf{y}, \tag{B.3}$$

where the r. h. s. of (B.3) tends to zero as $\varepsilon \to 0$. For the first integral on the r. h. s. of (B.2) the integration by parts gives

$$\begin{aligned}&\frac{i}{2\pi^2}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)}\frac{K_1(|\mathbf{y}|)}{|\mathbf{y}|}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\big(f(\mathbf{x}-\mathbf{y})\big)d\mathbf{y}\\ =&\frac{-i}{2\pi^2}\int\limits_{\mathbb{R}^3\setminus B(\varepsilon)}\boldsymbol{\alpha}\cdot\nabla_{\mathbf{y}}\Big(\frac{K_1(|\mathbf{y}|)}{|\mathbf{y}|}\Big)f(\mathbf{x}-\mathbf{y})d\mathbf{y}+\frac{iK_1(\varepsilon)}{2\pi^2\varepsilon}\int\limits_{\partial B(\varepsilon)}\boldsymbol{\alpha}\cdot\frac{\mathbf{y}}{|\mathbf{y}|}f(\mathbf{x}-\mathbf{y})d\mathbf{y}.\end{aligned} \tag{B.4}$$

We can rewrite the second integral on the r. h. s. of (B.4) as the sum of two integrals, using the Taylor expansion $f(\mathbf{x}-\mathbf{y}) = f(\mathbf{x}) - \nabla f(\mathbf{z})\cdot\mathbf{y}$ with $\mathbf{z}$ lying on the segment connecting $\mathbf{x}$ and $\mathbf{y}$. The integral containing $f(\mathbf{x})$ vanishes, because the function $\mathbf{y}|\mathbf{y}|^{-1}$ is odd. The integral with $\nabla f(\mathbf{z})\mathbf{y}$ is different from zero only for $\mathbf{x}$ in the compact region

$$\Omega := \big\{\mathbf{x}\big|\mathbf{x}\in\mathbb{R}^3,\ \mathrm{dist}\,\{\mathbf{x},\,\mathrm{supp}\,f\}\leqslant\varepsilon\big\}.$$

For $\mathbf{x}\in\Omega$ we have

$$\left|\frac{iK_1(\varepsilon)}{2\pi^2\varepsilon}\int\limits_{\partial B(\varepsilon)}\Big(\boldsymbol{\alpha}\cdot\frac{\mathbf{y}}{|\mathbf{y}|}\Big)\Big(\nabla f(\mathbf{z})\cdot\mathbf{y}\Big)d\mathbf{y}\right| \leqslant \frac{3K_1(\varepsilon)}{2\pi^2}\|\nabla f\|_\infty 4\pi\varepsilon^2. \tag{B.5}$$

Hence the last term on the r. h. s. of (B.4) converges to zero in the L_2–norm. Together with (B.1) — (B.4) and (A.2) this proves Lemma 10. •

C Proof of Lemma 9

Let $f\in L_2(\mathbb{R}^{3N})$, $\mathrm{supp}\,f\subset[-2R,2R]^{3N}$. Then

$$f(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}_+^{3N}} c_{\mathbf{k}}\prod_{i=1}^{3N}\varphi_{k_i}(x_i),$$

where

$$\varphi_k(x) = \begin{cases}\dfrac{1}{\sqrt{2R}}\sin\Big(\pi k\Big(\dfrac{1}{2}+\dfrac{x}{4R}\Big)\Big), & x\in[-2R,2R],\\ 0, & x\notin[-2R,2R],\end{cases}$$

$c_{\mathbf{k}}$ are the Fourier coefficients of $f|_{[-2R,2R]^{3N}}$.

For the Fourier transform of f we have

$$\hat{f}(\mathbf{p}) = \sum_{\mathbf{k}\in\mathbb{Z}_+^{3N}} c_{\mathbf{k}} \prod_{i=1}^{3N} \hat{\varphi}_{k_i}(p_i), \tag{C.1}$$

where

$$\hat{\varphi}_k(p) = \frac{4\sqrt{\pi R} k e^{i\frac{\pi}{2}(k-1)} \sin\left(\frac{\pi k}{2} - 2pR\right)}{\pi^2 k^2 - 16 p^2 R^2}. \tag{C.2}$$

Let

$$L := \frac{1536 RNM}{\pi^3} + 1. \tag{C.3}$$

Assume that f is orthogonal to the linear span of L^{3N} functions

$$\left\{ \prod_{i=1}^{3N} \varphi_{k_i}(x_i), \quad k_i \in [0, L-1] \cap \mathbb{Z}, \quad i = 1, \dots 3N \right\}.$$

Then the summation in (C.1) can be restricted to

$$\mathbf{k} \in \bigcup_{j=1}^{3N} \gamma_j, \quad \gamma_j := \bigcap_{l=1}^{j-1} \{\mathbf{k} \in \mathbb{Z}_+^{3N} | k_l < L\} \cap \{\mathbf{k} \in \mathbb{Z}_+^{3N} | k_j \geqslant L\}.$$

Obviously $\|\hat{f}\|^2_{L_2(\mathbb{R}^{3N})} = \sum\limits_{\mathbf{k}\in \bigcup\limits_{j=1}^{3N}\gamma_j} |c_{\mathbf{k}}|^2$. On the other hand,

$$\begin{aligned}
&\|\hat{f}\|_{L_2(W_M)} \leqslant \sum_{j=1}^{3N} \Big\| \sum_{\mathbf{k}\in\gamma_j} c_{\mathbf{k}} \prod_{i=1}^{3N} \varphi_{k_i}(p_i) \Big\|_{L_2(\{|p_j| \leqslant M\})} \\
&= \sum_{j=1}^{3N} \left(\sum_{\mathbf{k},\mathbf{k}'\in\gamma_j} \langle c_{\mathbf{k}}, c_{\mathbf{k}'} \rangle \int_{-M}^{M} \varphi_{k_j}(p_j) \overline{\varphi_{k'_j}(p_j)} dp_j \prod_{\substack{i=1 \\ i\neq j}}^{3N} \int_{\mathbb{R}} \varphi_{k_i}(p_i) \overline{\varphi_{k'_i}(p_i)} dp_i \right)^{1/2} \\
&= \sum_{j=1}^{3N} \left(\sum_{\substack{k_i=1 \\ i<j}}^{L} \sum_{\substack{k_i=1 \\ i>j}}^{\infty} \sum_{k_j, k'_j = L}^{\infty} \langle c_{(k_1,\dots,k_j,\dots,k_{3N})}, c_{(k_1,\dots,k'_j,\dots,k_{3N})} \rangle \int_{-M}^{M} \varphi_{k_j}(p) \overline{\varphi_{k'_j}(p)} dp \right)^{\frac{1}{2}}.
\end{aligned}$$

Since

$$k_j,\, k'_j \geqslant L > \frac{4\sqrt{2} MR}{\pi}, \tag{C.4}$$

we estimate

$$\Big|\int_{-M}^{M}\varphi_{k_j}(p)\overline{\varphi_{k'_j}(p)}dp\Big| \leqslant 16\pi Rk_jk'_j\int_{-M}^{M}\frac{1}{|\pi^2k_j^2-16p^2R^2||\pi^2k_j'^2-16p^2R^2|}dp$$

$$\leqslant 16\pi Rk_jk'_j\cdot 2M\cdot\frac{2}{\pi^2k_j^2}\cdot\frac{2}{\pi^2k_j'^2}=\frac{128RM}{\pi^3k_jk'_j}.$$

Applying the Schwarz inequality, we arrive at

$$\Big|\sum_{k_j,k'_j=L}^{\infty}\langle c_{(k_1,\dots,k_j,\dots,k_{3N})},c_{(k_1,\dots,k'_j,\dots,k_{3N})}\rangle\int_{-M}^{M}\varphi_{k_j}(p)\overline{\varphi_{k'_j}(p)}dp\Big|$$

$$\leqslant\frac{128RM}{\pi^3}\sum_{k'_j=L}^{\infty}|c_{(k_1,\dots,k'_j,\dots,k_{3N})}|^2\cdot\sum_{k_j=L}^{\infty}k_j^{-2}$$

$$\leqslant\frac{128RM}{\pi^3(L-1)}\sum_{k'_j=L}^{\infty}|c_{(k_1,\dots,k'_j,\dots,k_{3N})}|^2.$$

Therefore

$$\|\hat f\|_{L_2(W_M)}\leqslant\sum_{j=1}^{3N}\Big(\frac{128RM}{\pi^3(L-1)}\sum_{\mathbf{k}\in\gamma_j}|c_{\mathbf{k}}|^2\Big)^{1/2}$$

$$\leqslant\sqrt{\frac{384RNM}{\pi^3(L-1)}}\|\hat f\|_{L_2(\mathbb{R}^{3N})}=\frac{1}{2}\|\hat f\|_{L_2(\mathbb{R}^{3N})}.$$

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